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MOLECULAR DYNAMICS SIMULATION OF THE THERMAL TRANSPORT ON HOLEY COPPER SUBSTRATES

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ABSTRACT

Heat transfer in particular can be optimized by designing the macro-structure of the fluid-solid interface, which includes mounting pin-fins or acid etching of the surface. However, the mechanism behind heat transfer at the nanoscale is different from that at macroscale as the size of the surface structure reaches the phonon mean free path. While recent studies have considered the ballistic phonon transport in many nanoscale metallic materials, the relation between ballistic configuration and solid-liquid heat transfer is still limited. To this end, we investigate the effect of the nano hole on solid-liquid heat transfer using molecular dynamics simulations in the presence of nanoscale surface structures – here represented by nanoholes in the surface. As a result, the larger hole can enable a better capacity to water molecules for absorbing the energy from copper substrate. Therefore, the presence of the nanoholes results in a smaller temperature difference at the interface which enhances the solid-liquid heat transfer. Our results could provide the basis for further research on the thermal transport of bubble nucleation on nanostructures and could shed light on some principles behind the coupling of ballistic configuration and bubble nucleation.

INTRODUCTION

The bubble nucleation of water received significant attention with respect to improve heat transfer in thermal management system of micro-electric system, which is required for solving the safety issues of explosion and fire resulting from heat and mass transfer [1–3]. Moreover, with the rapidly growing list of applications of nanofluidic system, there is an increased interest on boiling and micro- and nanoscale. However, in contrast to macroscale cases, Fourier law describing heat transfer is known to fail for bubble

nucleation and its thermal transport [4, 5]. The size of the object structure is became the major factors that affect bubble conformations and nanoscale heat transfer [6, 7]. Several experimental and theoretical studies have been performed to understand the unique behaviour of heat transfer at nanoscale based on molecular dynamics simulation. Mukherjee and Datta [8] investigated the bubble nucleation on silicon substrates. They found that the rate of bubble growth is a function of notch height, notch width, notch type, and notch spacing on the uneven surface. Zhang [9] demonstrated the explosive boiling on a copper surface using the liquid argon as the working fluid. Their results showed that nanochannels can significantly facilitate the thermal energy transfer from the solid copper surface to the liquid argon. Diaz and Guo [10] showed that using nano bulges can

NOMENCLATURE

Φ_{ij}	[eV]	The pair potential interaction between atoms i and j
r_{ij}	[Å]	The distance between particles i and j
ρ_j	[e/cm ³]	Atomic electron densities
U_{ij}	[eV]	The Lennard-Jones 12-6 interaction and Coulombic potentials
σ_{ij}	[eV]	The distance parameters of the Lennard-Jones interactions
ε_{ij}	[Å]	The energy parameters of the Lennard-Jones interactions
q_j	[e]	The electric charge of particle j
F_i	[eV]	The embedding energy of atom i in the superposition of atomic electron densities $\rho_j(r_{ij})$
D	[Å]	The diameter of the nanohole
Subscripts		
Cu		Copper
O		Oxygen
H		Hydrogen
tot		Total
ij		Between particle i and particle j
i		Particle i
j		Particle j

enhance the heat transfer performance in overall boiling.

In these previous studies, the onset points of the bubble were triggered firstly by the presence of the hole on the substrate surface. Hence, the interest for the ballistic phonon transport in nanoscale holes has given rise to numerous studies. As reported by Lee et al. [11], the ballistic phonon via the hole path to surface region can carry heat without internal scattering when the size of the substrate is smaller than its phonon mean free path. In nanoconfinements, the ballistic phonon transport can domain the heat flow allowing to manipulation of the thermal transport which is of key importance for potential phononic applications [12, 13].

The phononic applications on fluids have not been widely explored because the inherent phonon scattering is a factor found to reduce thermal conductivity. Only recently, a novel investigation has demonstrated the effect of phonon-fluid coupling on energy dissipation [14]. They found that the phonon-fluid coupling strength and consequently the phonon relaxation times can be manipulated by changing the fluid density. In the other hand, Han and Merabia [15] have shown that nanoparticle can shift the liquid phonon from low to high frequencies, which leads to a better heat dissipation in liquids. With this in mind, the effect of phonon transport on bubble nucleation should be considered. Therefore, in this paper, we investigate the relationship between the bubble nucleation and the phonon transport on a copper substrate with holes and aims to provide some information. Our results provide insight into the coupling of ballistic phonon transport and bubble nucleation.

SIMULATION METHODOLOGY

Molecular dynamics simulations are performed for a solid-liquid system which consists of a solid copper substrate with or without different size holes and a water film in contact with the copper slab. A molecular simulation box with the length of 140Å, width of 140Å and height of 800Å is shown in Figure 1. The initial configuration of the simulation system comprised of 87025 water molecules and 50882 copper atoms. The copper atoms were arranged on a face-centered cubic (FCC) structure with the lattice constant of 3.61 Å. Besides, in order to avoid the migration and deformation of the solid wall, the two layers at the bottom of the copper substrate are kept fixed. The embedded atom model (EAM) was used to describe the interaction potential between copper atoms because it has shown good agreement with experimental results [16]. This interaction potential can be expressed as,

$$E_{tot} = \frac{1}{2} \sum \Phi_{ij}(r_{ij}) + \sum F_{ij}(\rho_{i,tot}), \rho_{i,tot} = \sum \rho_j(r_{ij}) \quad (1)$$

Here, $\Phi_{ij}(r_{ij})$ is the pair potential interaction between atoms i and j separated by a distance of r_{ij} . $F_{ij}(\rho_{i,tot})$ is embedding energy of atom i in the superposition of atomic electron densities $\rho_j(r_{ij})$.

Water molecules are described by the extended simple point charge (SPC/E) water model. The H-O-H angle and OH bond are 109.47° and 1 Å, respectively. The partial point charges for the oxygen and hydrogen atoms is $q_O = -0.8476e$ and $q_H = 0.4238e$. The interaction potential between the oxygen atoms involved the Lennard-Jones 12-6 interaction and Coulombic potentials [17], expressed as

$$U_{ij} = 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] + \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} \quad (2)$$

Where ϵ_0 is the vacuum permittivity. Moreover, σ_{ij} and ε_{ij} are the distance and energy parameters of the Lennard-Jones interactions, respectively. Here, the distance and energy parameters of Lennard-Jones interactions for oxygen atoms are considered to be $\varepsilon_{O-O} = 0.0067389eV$ and $\sigma_{O-O} = 3.166\text{Å}$, and no Lennard-Jones potential between hydrogen and oxygen atoms ($\varepsilon_{H-H} = 0.0eV$, $\sigma_{H-H} = 0.0\text{Å}$, $\varepsilon_{O-H} = 0.0eV$, $\sigma_{O-H} = 0.0\text{Å}$). Moreover, Lennard-Jones 12-6 interaction was applied to describe the copper-water interaction, the distance and energy parameters are $\varepsilon_{Cu-O} = 0.0524eV$ and $\sigma_{Cu-O} = 2.7519\text{Å}$ [17].

This simulations in the present work were carried out using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). The periodical boundary conditions are applied to all three direction of the box. The motion equations are integrated in time using a time step of 2 fs. The bond length and angle of the water molecules are maintained by applying the SHAKE algorithm [18]. And the particle-particle-mesh (PPPM) method [19] was used to modify the long-range Coulombic interaction with a accuracy of 10^{-6} . Initially, the system was equilibrated at a temperature of 298.15 K for 50000 steps in NVT ensemble. To ensure the system reaches the equilibrium state, it was run for 60000 steps in the NVE ensemble. After equilibration is reached, the atoms in the top layer were kept at 500 K by using the Nose-Hoover thermostat for running 500000 steps. The thermal and physical parameters, including temperature, heat flux and velocity autocorrelation function were calculated for different reference cases. In the simulations, these parameters were computed from atomic trajectories extracted each 1 ns.

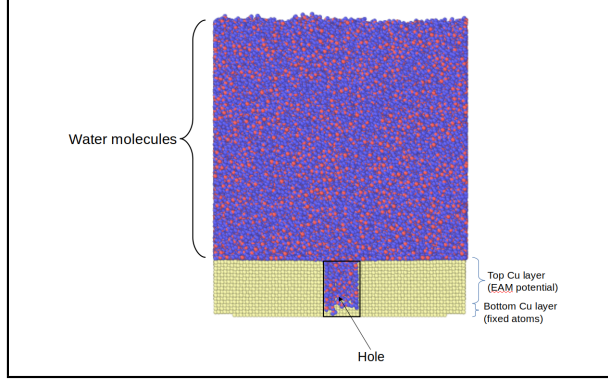


Figure 1: The schematic diagram of the simulation system

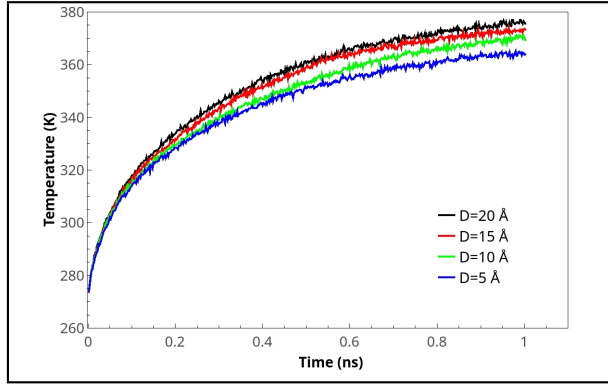


Figure 2: The temperature variation of the water region in four cases with different hole diameter

RESULTS AND DISCUSSION

Figure 2 shows the temperature variation of the water region in the course of simulation for the four cases with different diameter of the holes ($D=5, 10, 15$ and 20 Å). It can be found that the temperature of the water region after the simulation was up to 363.88, 369.41, 373.31 and 375.60 K, respectively. For these four cases, with the increase of the hole diameter, the larger aperture can transfer the heat to the water region faster, which leads to the less time for the same operating temperature range. It should be pointed out that the increase rate of temperature between the cases of 20 Å and 15 Å slows down compared to that of 15 Å and 10 Å cases.

As shown in Figure 3, the temperature difference of the water region for the cases of 20 Å and 5 Å is close to that between 15 Å and 5 Å cases, indicating that the growth rate of the water temperature is a non-linear relationship to the increase of the hole diameter. Indeed, when the diameter of the hole exceeds a certain value, its effect on increasing the temperature of the water region is not obvious, even

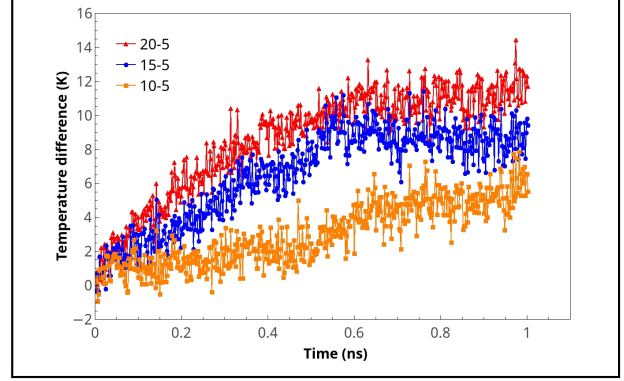


Figure 3: The temperature difference of the water region for three cases (10 Å , 15 Å and 20 Å) compared to the case of 5 Å

impedes the heat transfer. In other word, the energy absorption would be mitigated during the simulation process.

In addition, for the holes of 15 Å and 20 Å , they led to the shorter time for heating the water region to the same temperature point within 1 ns, indicating the water region in this cases absorbed the energy from copper substrate more effectively. Figure 4 shows the dependence of the total energy difference between the copper substrate and the water region in this simulation system on the simulation time for the four cases ($D=5, 10, 15$ and 20 Å). In the early time of running, the energy difference between the copper substrate and water region increases dramatically due to the water molecules absorb the energy from the copper heating layers. Then, the variation of the energy difference slows down with the running time. This results from the increasing temperature of the water region which reduces the temperature difference of the copper and water region gradually. A low temperature difference retarded the heat transfer from copper substrate to water region. On the other hand, it can be found that the energy difference decreases with the increase of the hole diameter. In the whole process, the case with the diameter of 20 Å keeps the lowest energy difference. This indicates that the hole with a larger diameter can improve the energy transfer from the copper to the water region, which results to the effective heat transfer, especially for the vibrating water molecules. As shown in Figure 5, the water molecules collect the potential and kinetic energy from the copper atoms to push its total energy dramatically in the early of the running. As time goes by, the weakened energy transmission slowed down the increase of the water total energy. It is in a well agreement with the temperature variation of the water region in Figure 2. In a word, the difference of the hole diameter leads to the lower energy

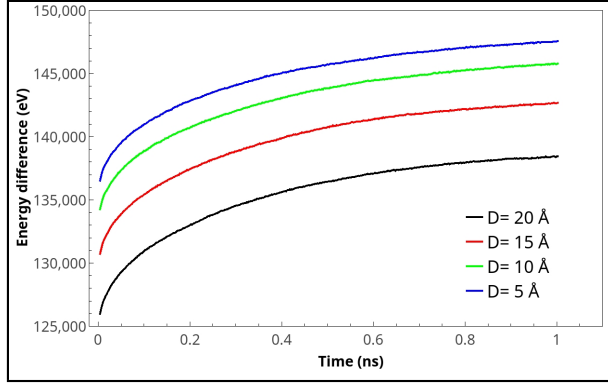


Figure 4: The comparison of the total energy difference between the copper and the water region for four cases

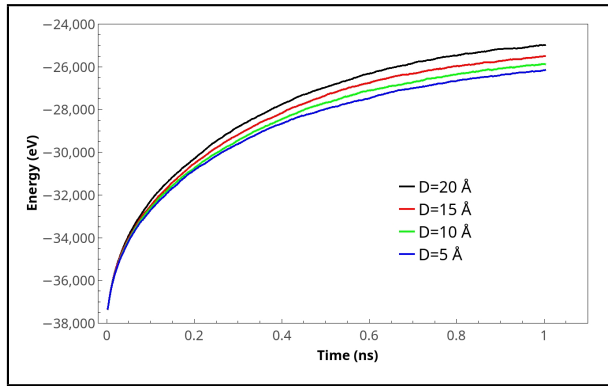


Figure 5: The comparison of the water energy for four cases

difference of copper substrate and water region in the process of solid-liquid heat transfer, as well as giving a better capacity for absorbing the energy from copper substrate.

CONCLUSION

Preliminary molecular dynamics simulations have been performed to study the thermal transport on the solid-liquid system with copper substrate and water region has been studied based on different holes. The thermal properties and phonon transport characteristics of the system, including the copper substrate and water region are evaluated and compared under the heating temperature of 500 K. The results indicate that the presence of the holes facilitate the heat transfer from copper substrate to water region for all cases studied. It was found that the hole in the copper substrate have a significant influence on the enhancement of heat transfer between copper wall and water region. Moreover, the enhancement increases with the increasing hole diameter in a certain range. The temperature of the water region increase faster in the case with a larger hole. Besides,

the temperature difference associated with the copper substrate and water area reduced with the increase of the hole diameter. More than this, the difference of the hole diameter leads to the lower energy difference of copper substrate and water region in the process of solid-liquid heat transfer, as well as giving a better capacity for absorbing the energy from copper substrate.

References

- [1] R. Wen, Q. Li, W. Wang, B. Latour, C. H. Li, C. Li, Y.-C. Lee, and R. Yang, "Enhanced bubble nucleation and liquid rewetting for highly efficient boiling heat transfer on two-level hierarchical surfaces with patterned copper nanowire arrays," *Nano Energy*, vol. 38, pp. 59–65, 2017.
- [2] E. V. Levine, M. M. Burns, and J. A. Golovchenko, "Nanoscale dynamics of joule heating and bubble nucleation in a solid-state nanopore," *Physical Review E*, vol. 93, no. 1, p. 013124, 2016.
- [3] A. Cowley, D. Maynes, J. Crockett, and B. D. Iverson, "Bubble nucleation in superhydrophobic microchannels due to subcritical heating," *International Journal of Heat and Mass Transfer*, vol. 121, pp. 196–206, 2018.
- [4] A. Rana, R. Ravichandran, J. Park, and R. Myong, "Microscopic molecular dynamics characterization of the second-order non-navier-fourier constitutive laws in the poiseuille gas flow," *Physics of Fluids*, vol. 28, no. 8, p. 082003, 2016.
- [5] A. Singh and E. B. Tadmor, "Thermal parameter identification for non-fourier heat transfer from molecular dynamics," *Journal of Computational Physics*, vol. 299, pp. 667–686, 2015.
- [6] Y. Gao, Q. Liu, and B. Xu, "Lattice mismatch dominant yet mechanically tunable thermal conductivity in bilayer heterostructures," *ACS nano*, vol. 10, no. 5, pp. 5431–5439, 2016.
- [7] S. Shin, G. Choi, B. Rallabandi, D. Lee, D. I. Shim, B. S. Kim, K. M. Kim, and H. H. Cho, "Enhanced boiling heat transfer using self-actuated nanobimorphs," *Nano letters*, vol. 18, no. 10, pp. 6392–6396, 2018.
- [8] S. Mukherjee, S. Datta, and A. K. Das, "Molecular dynamic study of boiling heat transfer over structured surfaces," *Journal of Heat Transfer*, vol. 140, no. 5, p. 054503, 2018.

- [9] S. Zhang, F. Hao, H. Chen, W. Yuan, Y. Tang, and X. Chen, “Molecular dynamics simulation on explosive boiling of liquid argon film on copper nanochannels,” *Applied thermal engineering*, vol. 113, pp. 208–214, 2017.
- [10] R. Diaz and Z. Guo, “A molecular dynamics study of phobic/philic nano-patterning on pool boiling heat transfer,” *Heat and Mass Transfer*, vol. 53, no. 3, pp. 1061–1071, 2017.
- [11] J. Lee, J. Lim, and P. Yang, “Ballistic phonon transport in holey silicon,” *Nano letters*, vol. 15, no. 5, pp. 3273–3279, 2015.
- [12] N. Li, J. Ren, L. Wang, G. Zhang, P. Hänggi, and B. Li, “Colloquium: Phononics: Manipulating heat flow with electronic analogs and beyond,” *Reviews of Modern Physics*, vol. 84, no. 3, p. 1045, 2012.
- [13] M. Maldovan, “Sound and heat revolutions in phononics,” *Nature*, vol. 503, no. 7475, p. 209, 2013.
- [14] S. De and N. R. Aluru, “Energy dissipation in fluid coupled nanoresonators: The effect of phonon-fluid coupling,” *ACS nano*, vol. 12, no. 1, pp. 368–377, 2018.
- [15] H. Han, S. Merabia, and F. Müller-Plathe, “Thermal transport at a solid–nanofluid interface: from increase of thermal resistance towards a shift of rapid boiling,” *Nanoscale*, vol. 9, no. 24, pp. 8314–8320, 2017.
- [16] H. H. Wu and D. R. Trinkle, “Cu/ag eam potential optimized for heteroepitaxial diffusion from ab initio data,” *Computational Materials Science*, vol. 47, no. 2, pp. 577–583, 2009.
- [17] B.-B. Wang, Z.-M. Xu, X.-D. Wang, and W.-M. Yan, “Molecular dynamics investigation on enhancement of heat transfer between electrified solid surface and liquid water,” *International Journal of Heat and Mass Transfer*, vol. 125, pp. 756–760, 2018.
- [18] J. Beckers, C. Lowe, and S. De Leeuw, “An iterative ppm method for simulating coulombic systems on distributed memory parallel computers,” *Molecular simulation*, vol. 20, no. 6, pp. 369–383, 1998.
- [19] J.-P. Ryckaert, G. Ciccotti, and H. J. Berendsen, “Numerical integration of the cartesian equations of motion of a system with constraints: molecular dynamics of n-alkanes,” *Journal of computational physics*, vol. 23, no. 3, pp. 327–341, 1977.